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Comparison of particle placement schemes for discrete element models

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Abstract: The estimation of uncertainties in probabilistic structural analysis may improve if the spatial variability concept is properly introduced. The presented paper addresses various discrete particle placement choices and schemes for discrete particle models such that the governing realization of random fields for spatially variable material properties is correlated to a particular structural discretization (i.e. radius and placement of particles) in a discrete framework. Although some discrete element models already mimic microstructural effects of concrete very well, when compared to the continuum framework, there are still reasons for introducing higher order spatial variability, such as the statistical size effect that cannot be captured numerically without introducing spatial variability in the material property fields with an appropriately chosen auto-correlation length. By introducing the newly developed spatial variability package, classical experiments for concrete may be more realistically reproduced and associated statistical features discussed, also in terms of particular particle placement schemes, observed scattering and physical reference.

1 Introduction

Recent developments in particle placement schemes for the lattice discrete particle modelling (LDPM) [1]–[3] are presented in this paper as one of the essential components of probabilistic structural analysis and uncertainty quantification. In this context, the random field and spatial variability concepts in general are frequently adopted in order to account for the fluctuations of material characteristics on scales independent of the geometrical characterization of the mesostructure as represented by particular particle configurations mimicking the aggregate placement. The original LDPM modelling paradigm naturally accounts for material heterogeneity by randomly placed particles with diameters randomly sampled from a fuller curve and filling a required volume fraction. Although this method proves to be sufficient for some application domains, the authors believe that the LDPM realism may be enhanced by introducing correlated particle placement schemes, which would enable to control and interpret the response scatter.

2 LDPM

A well-established member of the discrete framework, the lattice discrete particle model (LDPM) has been extensively calibrated and validated and it has shown superior capabilities in reproducing and predicting concrete behaviour. It simulates the mesostructure of concrete by a three-dimensional (3D) assemblage of particles (fig. 1) that are generated randomly according to a given grain size distribution. Delaunay tetrahedralization and 3D domain tessellation are used here to generate a system of cells interacting through triangular facets. Displacements and rotations of such adjacent particles form the discrete compatibility equations in terms of rigid body kinematics. At each cell facet the mesoscale constitutive law is formulated such that it simulates cohesive fracture, compaction due to pose collapse, frictional slip and rate effect. For each single particle an equilibrium equations are finally formulated. An extended version of LDPM is currently developed and simulates various coupled deterioration mechanisms, such as Alkali-Silica reaction (ASR) [3], [4]. A further development is the age-dependent LDPM framework in which the local material properties are derived by chemo-mechanical coupling with a chemo-hygro-thermal model [5] which also drives the creep and shrinkage analysis in a rate type form [6].

3 Stochastic framework

The uniqueness of each LDPM realization may be mostly attributed to the initial randomized particle generation, assuming deterministic boundary conditions and insignificant solver noise. In the context of engineering risk analyses, where structural models typically do not have a closed-form solution and a single evaluation is already computationally demanding, the requirement is to reproduce the statistical characterization of the response quantities. In some cases, the sensitivity of response to individual input parameters, such as material, technological or environmental characteristics can be estimated by the deterministic study of the problem (identify unfavourable conditions) and a sampling strategy can be effectively formulated. This is routinely done e.g. in structural static analysis with randomized scalar input variables, such as material parameters [7]–[9]. Such approach yields reasonable results in terms of accuracy and computational cost, unless due to a high number of random input variables, an extremely complex (or ill-defined) structural model, or simply due to solver noise, the particular input-output dependency becomes non-monotonous [10].

The importance of spatial variability in structural safety is indicated by a growing number of publications; however, effective sampling strategies are yet to be established [11]. Unlike in the previous case of scalar random input variables, the sensitivity of individual input patterns (random fields) cannot be obtained by a deterministic study of the problem and the likelihoods cannot be easily assigned to individual realizations of such patterns due to obvious reasons [12]. Here it should be noted that in most cases the spatial heterogeneity at arbitrary scale (meso, micro and macro) is irrelevant for the assessment of engineering structures made from basic construction materials, such as concrete, steel or wood. However, it becomes highly relevant to currently designed composites [13], structural details such as those of anchoring technology [14] or geotechnical assessment [15]. Similarly, the implicit treatment of spatial variability is important to the reliability based code calibration [16], [17], design of experiments [18] and verification of various hypotheses or limit theorems, such as fracture behaviour or size effect [14], [19].

3.1 Implementation of spatially variable fields

A spatial variability package has been developed by the authors for the LDPM, implemented in the solver MARS (Multiscale-multiphysics Analysis of the Response of Structures) [20], [21], which includes spectral representations of random fields (Gaussian and non-Gaussian; fig. 1), gradient-based fields (fig. 2) and an equation interpreter for arbitrary matrix algebraic operations. This unique package further includes various particle placement schemes, as introduced in the next chapter, some of which may utilize the resulting random field or a combination of several random fields. This way, inherent variability, construction process, such as concrete casting, and transport processes (such as e.g. diffusion) may be experimentally investigated in the multiscale-multiphysics framework.

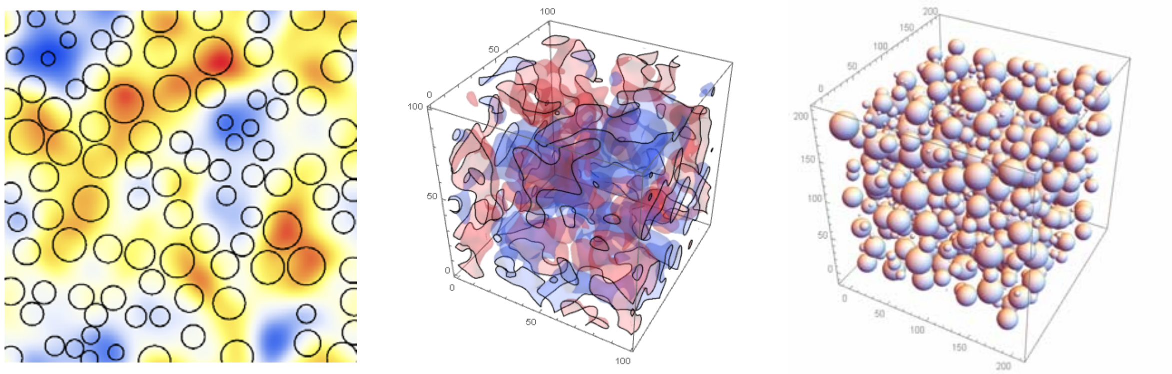

Figure 1: Example of particle placement and size governed by random field in 2D (left), realization of random field in 3D (center) and particles correlated to this random field (size, position), following a fuller grading curve (size) and filling a 30% volume (right).

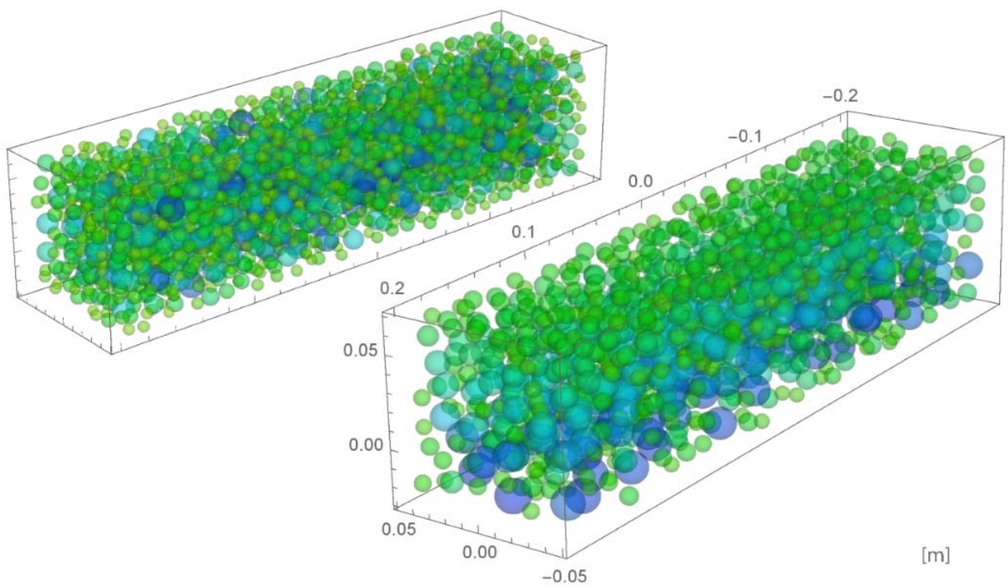

Figure 2: Comparison of IRPP (top- left) and gradient-based field (bottom-right) simulating the effect of gravity during castig process, both following a fuller grading curve (size) and filling a 30% volume (right).

4 Placement schemes and material characterization

The proposed particle placement schemes may significantly influence the scattering and asymptotic properties of the spatially variable models and thus contribute to the general understanding of the physics and reliability of spatial variability.

The abstraction levels for LDPM are categorized as following.

4.1 Independent and random particle placement

Independent and random particle placement (IRPP) and random diameter according to the size distribution curve and required volume fraction, as is currently implemented in the LDPM. No conflicting requirements are to be solved. Overlapping or less than minimum distance particles are resamples. Implications are scarcely populated boundary regions and invariant coefficient of variation, typically around 4.5% for classical concrete experiments (three point bending test), which is less than observed. The original procedure for generating particles is described in detail in [1].

4.2 IRPP combined with random or gradient-based field for material characterization only

The second abstraction level assumes the original particle placement scheme, i.e. the IRPP, combined with one or more random fields, which is used to describe material local fluctuations of material properties resulting from inherent variability (random field) and construction or transport processes (gradient-based fields). Similarly to the previous case, there are no geometry-related conflicting requirements and overlapping or less than minimum distance particles are resampled. Boundary regions may be normally populated by adopting a simple modification to the re-sampling algorithm.

Material characterizations derived from random fields must be verified for inadmissible values, such as negative strength, modulus, etc. This may lead to a conflict if the governing probability distribution used for generating the random field is to be maintained. Otherwise, truncated distributions may be used or the realization of random field can be rescaled to fit admissible range [11], [22], [23].

4.3 Particle generation governed by initial random or gradient-based field

Here it is assumed that an initial random or gradient-based field of choice (or their arbitrary combination) is governing not only the material properties, but also the particle generation process (i.e. the position and/or the size of each particle). If particle generation is to be governed not only by granulometric distributions, but also by an initial random or gradient-based field, the particle generation becomes a complex problem and has to be approached by balancing trade-offs between conflicting goals. Clearly, the global requirement on particular size distribution can lead to a local conflict with the initial random field, the role of which can be further ambiguous if we consider it to affect both the position and size of the particles (clustering of large particles). Details regarding the associated steps/choices for random fields were published in [24]. For higher volume fractions this becomes a computationally expensive procedure, however local conflicts can be resolved in parallel and terminate with the first valid particle. The advantage of the approach lies in the compatibility of the mimicked meso-structure with the material property fields which otherwise cannot be maintained. This implies a causal relationship between spatial variability, auto-correlation length of the random fields, type of spectral function and meso/micro-structure of the material which is an open research question.

5 Discussion

A spatial variability package for LDPM has been presented, including two new abstraction levels for LDPM, where material characterization and/or particle generation are governed by an initial random field, which increases the consistency of the LDPM modelling paradigm and potentially enhances the realism of the LDPM simulations, if properly understood. This, however, requires addressing several milestones, such as:

- Establishing a physical reference for the governing random field model, in particular the choice of spectral function, its parameters and relationship to correlation length.
- Introducing and combining different sources of spatial variability, i.e. not only material parameters, but also the construction and diffusion/transport processes.
- Objective statistical characterization of spatially variable LDPM models in a small sample Monte Carlo simulation framework.

Addressing such high-dimensional problems will not be possible in the near future without massive parallelisation of the associated tasks and utilization of scientific clusters. In order to introduce spatial variability into structural reliability, some preliminary work of [11], [12] on identification strategy for correlated random processes may be further utilized for LDPM models, realizations of which may be further classified by the resulting correlation structure. In this way, various particle placement schemes may not only be statistically benchmarked, but also characterized in terms of first passage probabilities or probability distributions, given a set of critical criteria for a particular model.

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